



chain nodes :

7 8 9 10 11 12 13 14 19 20 21 22 23 24 25 26 27 28 29 30 31

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 1-8 2-11 3-23 4-9 4-10 5-13 6-26 11-12 12-19 12-22 13-14 14-20 14-21 23-24  
24-25 24-29 26-27 27-28 29-30 29-31

ring bonds :

1-2 1-3 2-3 4-5 4-6 5-6

exact/norm bonds :

1-2 1-3 1-7 1-8 2-3 4-5 4-6 4-9 4-10 5-6 12-19 12-22 14-20 14-21 29-30 29-31

exact bonds :

2-11 3-23 5-13 6-26 11-12 13-14 23-24 24-25 24-29 26-27 27-28

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS  
25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

fragments assigned product role:

containing 4

fragments assigned reactant/reagent role:

containing 1